GBTOXe Users' Manual

Prepared for:

ThermoRetec
St.Paul, MN

Prepared by:

HydroQual
Mahwah, NJ

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PREFACE

The Lower Fox River/Green Bay ecosystem was extensively studied as part of the 1989-90 GBMBS (USEPA 1989; USEPA 1992a,b). As part of that study, a suite of coupled water quality models describing PCB transport in the Lower Fox River and Green Bay were developed. In that effort, Three generations of water quality model development have been initiated. The initial models calibrated to GBMBS conditions represent the first generation of model development for the Green Bay portion of the project area (Bierman et al. 1992). The re-calibration of that model to better reflect solids dynamics in the bay represents the second generation of development (DePinto et al. 1993). The model developed as part of RI/FS efforts is the result of continued assessments of Green Bay water quality model performance and represents the third generation of model development. To distinguish it from prior generations of development, the third generation model is identified as the “enhanced” Green Bay Toxics model (GBTOXe).

Like the previous generations of Green Bay water quality model development, The GBTOXe model framework is based on WASP5 but with modifications to accommodate information and conditions specific of Green Bay. Since many of the WASP5 format requirements for the input file are maintained in GBTOXe, this document is a copy of the WASP5 input dataset manual (Part B of The Water Quality Analysis Simulation Program documentation, Ambrose, et al., 1993) with additional text (bold) outlining the requirements to create a GBTOXe input file. The purpose of this manual is only to offer guidance on how to build or revise a GBTOXe input file. Any descriptive text not pertinent to an implementation of the current version of GBTOXe was removed.

GBTOXe is a work in progress. Its design is highly structured for application to Green Bay and should not be considered a general use water quality model. While every attempt was made to ensure that the model functions as intended, there is no guarantee that the code is bug free. Some of the options available in WASP and GBTOX have been disable or if selected will produce run-time errors. Option selections that are known to cause run-time errors are noted in the manual.

CHAPTER 1

INTRODUCTION

1.1 GENERAL CONSIDERATIONS

This section describes the input required to run the GBTOXe water quality program. Like WASP5, GBTOXe data are divided into 10 groups, A through J:

A - Model Identification and Simulation Control

B - Exchange Coefficients

C - Volumes

D - Flows

E - Boundary Concentrations

F - Waste Loads

G - Environmental Parameters

H - Chemical Constants

I - Time Functions

J - Initial Conditions

The following is a brief explanation of each data group:

DATA GROUP A provides for descriptive model identification and contains simulation control options. The user must specify the number of segments and the number of systems. The user must also specify calculational time steps and print intervals here.

DATA GROUP B contains dispersive exchange information. Dispersion occurs between segments and along a characteristic length.

DATA GROUP C supplies initial segment volume information, and information on the segment type and underlying segment numbers. Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow. These values are used in reaeration and volatilization calculations only (not in the basic transport calculations).

DATA GROUP D supplies flow and sediment transport information between segments. Currently, the flows input dataset must be

imported from an external hydrodynamic file.

DATA GROUP E supplies concentrations for each system at the boundaries. All system concentrations must be supplied for each boundary. Boundary concentrations vary with time in a piecewise linear time function.

DATA GROUP F defines the waste loads and segments that receive the waste loads for both point and diffuse sources. Point source loads vary with time in a piecewise linear time function. Non-point source loads vary with time in a daily step function.

DATA GROUP G contains appropriate environmental characteristics of the water body. These parameters are spatially variable, varying with each model segment.

DATA GROUP H contains appropriate chemical characteristics or constants. Constants remain constant in both time and space.

DATA GROUP I contains appropriate environmental or kinetic time functions.

DATA GROUP J contains initial concentrations for each segment and each system, along with dissolved fractions and the density of solids systems.

The input dataset is a formatted ASCII file. The user must carefully place input data in the appropriate fields, and be sure to right justify integers.

The 6 systems for toxicant modeling are chemical 1, chemical 2, chemical 3, solids fraction 1, solids fraction 2, solids fraction 3, and solids fraction 4.

CHAPTER 2

DATA GROUP A: MODEL IDENTIFICATION AND SIMULATION CONTROL

Basic simulation information is provided in Data Group A, beginning with titles and descriptions in Records 1 and 2. The number of systems (state variables) and segments are specified in Record 4. Calculational time steps are provided in Records 6 and 7, and print intervals in Records 8 and 9. System bypass options are set in Record 10.

2.1 RECORD FORMATS

Record 1--Title of Simulation (A5, A75)

SIMTYP	=	type of simulation; TOXI4 = toxics dataset; EUTRO = eutrophication dataset. (A5)
TITLE1	=	descriptive title of simulation. (A75)

Record 2--Description of Simulation (A80)

TITLE2	=	description of simulation. (A80)

Record 3--Record 4 Names (A80)

HEADER	=	names of Record 4 variables, positioned properly; for user convenience only. (A80)

Record 4--Simulation Control Parameters (7I5, 2F5.0, F3.0, F2.0)

NOSEG	=	number of segments in model network. (I5)
NOSYS	=	number of model systems (state variables). (I5)
ICFL	=	flag controlling use of restart file; 0 = neither read from nor write to restart file (initial conditions located in input file); 1 = write final simulation results to restart file (initial conditions located in input file); 2 = read initial conditions from restart file created by earlier simulation, and write final simulation results to new restart file. (I5)
MFLAG	=	flag controlling messages printed on screen during simulation; 0 = all messages printed; 1 = simulation time only printed; 2 = all

messages are suppressed. (I5)

JMASS = system number for which mass balance analysis will be performed; 0 = no mass balance table generated. (I5)

NEGSLN = negative solution option; 0 = prevents negative solutions; 1 = allows negative solutions. (I5)

INTYP = time step option; 0 = user inputs time step history; 1 = model calculates time step. (I5)

ADFAC = advection factor; 0 = backward difference; 0.5 = central difference; 0-0.4 recommended. (F5.0)

ZDAY = day at beginning of simulation; 1 is first day. (F5.0)

ZHR = hour at the beginning of simulation. (F3.0)

ZMIN = minute at the beginning of simulation. (F2.0)

IDSY = system number of the concentration displayed at runtime(I5)

IDSG1 = Segment number for which the IDSY concentration will be displayed at runtime. (I5)

IDSG2 = Segment number for which the IDSY concentration will be displayed at runtime. (I5)

TADJ = factor by which input kinetic rates will be adjusted; 0 or 1.0 will cause no adjustment; 24.0 will adjust input rates in $hours^{-1}$ to $days^{-1}$. 86400.0 will adjust input rates in $seconds^{-1}$ to $days^{-1}$ (f10.0)

Record 5—Spatial and temporal averaging options (2I5, f10.0)

ISAVGOPT = Spatial averaging flag; 0 = no spatial averaging; 1 = compute spatial averages for specified segments (see records ?-?). IF ITAVGOPT (record 6) = 0 then instantaneous spatial averages will be computed and written to (?).out.

ITAVGOPT = Temporal averaging flag; 0 = no temporal averaging; 1 = compute temporal averages of the spatial averages of the specified segments (see records ?-?) over an averaging period of AVGPERIOD. Temporal averages of the spatial averages will be computed and written to (?).out. Note: ISAVGOPT must = 1 to obtain temporally averaged results (i.e., GBTOXE does not compute temporal averages for individual segments). IF ISAVGOPT = 0, ITAVGOPT and AVGPERIOD have no effect.

AVGINT = Interval in days over which temporal averages are to be computed. If ITAVGOPT = 0, AVGPERIOD has no effect.

IF ISAVGOPT = 0, skip records 7-9 and continue with record 10

Record 7--Number of Zones for which spatial averages will be computed (I5)

NCELLBLKS = number of zones.

Records 8-9 are repeated NCELLBLKS times.

Record 8—Number of Segments per zone (I5, a20)

NCELLS(IBLCK) =number of segments assigned to zone IBLCK where IBLCK = 1 to NCELLBLKS. Although not required, segments that are assigned to a zone should be vertically and horizontally contiguous.

ZONENAME(IBLK)=Name of zone.

Record 9--Segments assignment to zone IBLCK (16I5)

IBLKSEG(ICELL,IBLCK) = Segment assigned to zone IBLCK where ICELL = 1 to NCELLS(IBLCK)

Record 9 is repeated NCELLS(IBLK) / 16 times.

Note: Currently, GBTOXE is hardwired to output averaged results in a format that requires specific ordering of the zones: zone blocks 1, 6, 11, … must be water column only.

Zone blocks 2,3,4,5…7,8,9,10…etc must be segments in sediment layers 1,2,3,4 respectively.

Record 10--Number of Time Steps (I5)

NOBRK = number of different model time steps (I5)

Record 11--Time Steps (4(F10.0, F10.0))

DTS(I) = time step to be used until time T(I), minutes. (F10.0)

T(I) = time up to when time step DTS(I) will be used, days. (F10.0)

Record 12--Number of Print Intervals (I5)

NPRINT = number of print intervals. (I5)

Record 13--Print Intervals (4(F10.0, F10.0))

PRINT(I) = print interval to be used until time TPRINT(I), days. (F10.0)

TPRINT(I) = time up to when print interval PRINT(I) will be used, days. (F10.0)

Record 14--System Bypass Options (16I5)

SYSBY(K) = bypass option for system K; 0 = system will be simulated; 1 = system will be bypassed. (I5)

CHAPTER 3

DATA GROUP B: EXCHANGE COEFFICIENTS

Exchange coefficients for surface water and pore water are computed from input dispersion coefficients, cross-sectional areas, and characteristic lengths. Dispersion coefficients may vary in time according to piecewise-linear time functions, with groups of segment pairs having the same dispersion time function. Exchange data are read for each exchange field. Field one contains dispersion coefficients for water column exchanges. Field two contains exchange data for pore water exchange.

3.1 RECORD FORMATS

Record 1--Number of Exchange Fields (I5, 75X)

NRFLD = number of exchange fields. NRFLD will generally equal 2 for water column and pore water exchanges. (I5)

TITLE = name of data group. (75X)

If no exchange rates are to be read, set NRFLD to zero and continue with Data Group C. If only surface water exchanges are to be read, set NRFLD to 1 and input the proper values in records 2-6 and 12. If pore water exchanges are to be read, set NRFLD to 2 and input the proper values in records 2-12.

Record 2-- Exchanges Input File (a40,i2,f10.0)

HYDROFIE = Name of Exchanges File.

IRFILTYPE = File type; 0 = binary; 1= ASCII.

RWDTIME(1)= Time in days at which exchange file will rewind.

Currently, the user must make an entry for record 2 even if it not to be used. To use an external file as specified in record 2, set NTEX(1) = -6 in record 4 and skip to record 9. To bypass, follow specifications of records 4-8 as usual. GBTOXE currently reads Binary exchange files only.

The required format for the exchange file is a follows.

Initial read statements:

```
READ NTEX(1)                    !(Number of exchange pairs)
READ (IR(I),JR(I),I=1,NTEX(1)) !(I,J exchange pairs)
READ TIME                       !(time in days)
```

IMPORTANT! GBTOXE expects TIME to be double precision.

Subsequent read statements:

Throughout the simulation, GBTOXE compares the current run time with the last time break read in. When the run-time exceeds the time break the next set of exchanges, areas, and effective lengths are read in along with the next time break. The format below should be repeated for the number of time breaks desired:

```
READ (br(I),I=1,NTEX(1))       !(exchanges in m3/sec)
READ (a(I) ,I=1,NTEX(1))       !(area in m2)
READ (el(I),I=1,NTEX(1))       !(effective length in m)
READ TIME                      !(time to next break)
```

Note that exchanges are read in as Bulk dispersion rather than in L^2/T units. Nevertheless, a and el are still required.

Record 3—Vertical and Horizontal scale Factor (2F10.0)

SCALRV = Vertical scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor.

SCALRH = Horizontal scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor.

Record 4--Exchange Time Functions for Surface Water Field (I5, 2F10.0)

NTEX(1) = number of exchange time functions for field 1. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor. (F10.0)

CONVR = conversion factor for exchanges in field 1. (F10.0)

To skip surface water exchange field, set NTEX(1) to zero and continue with the pore water exchange field (record 7) or the exchange bypass options (record 12).

Records 3-6 are input as a group NTEX(1) times:

Record 5--Exchange Data (I5)

NORS(1,NT) = number of exchanges for field 1, time function NT. (I5)

Record 6--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K. (F10.0)

EL(K) = characteristic length in meters for exchange pair K. (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant. (2I5)

Record 4 is repeated NORS(1,NT) times.

Record 7--Number of Breaks in Time Function (I5)

NBRKR(1,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function. (I5)

Record 8--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in m^2/sec at time TR(K). (F10.0)

TR(K) = time in days. (F10.0)

Record 6 is repeated NBRKR(1,NT)/4 times.

Record 9--Exchange Time Functions for Pore Water Field (I5, 2F10.0)

NTEX(2) = number of exchange time functions for field 2. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 2 will be multiplied by this factor. (F10.0)

CONVR = conversion factor for exchanges in field 2. (F10.0)

To skip pore water exchange field, set NTEX(2) to zero and continue with record 12.

Records 8-11 are input as a group NTEX(2) times:

Record 10--Exchange Data (I5)

NORS(2,NT) = number of exchanges for field 2, time function NT. (I5)

NT = 1, NTEX(2)

Record 11--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K. (F10.0)

EL(K) = characteristic length in meters for exchange pair K. (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant. (2I5)

Record 9 is repeated NORS(2,NT) times.

Record 12--Number of Breaks in Time Function (I5)

NBRKR(2,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function. (I5)

Record 13--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in m^2/sec at time TR(K). (F10.0)

TR(K) = time in days. (F10.0)

Record 11 is repeated NBRKR(2,NT)/4 times.

Record 14--Exchange Bypass Options (16I5)

RBY(K) = exchange bypass option for system K; 0 = exchange occurs in system K; 1 = bypass exchange for system K. (I5)

K = 1, NOSYS

CHAPTER 4

DATA GROUP C: VOLUMES

Initial segment volumes are provided in Data Group C. In addition, segment type and underlying segment numbers are specified. Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow. These values are used in reaeration and volatilization calculations only (not in the basic transport calculations.)

4.1 RECORD FORMATS

Record 1--Preliminary Data (2I5, F10.0, 60X)

IVOPT = water column volume option -- 1 = constant water column volumes; 2, 3 = volumes adjusted to maintain flow continuity. (I5)

IBEDV = benthic volume option -- 0 = constant bed volumes; 1, bed volumes change in response to sediment transport. (I5)

TDINTS = benthic time step in days for recomputing porosity (if IBEDV = 0) or for sediment bed compaction (if IBEDV = 1). (F10.0)

TITLE = name of data group. (60X)

Record 2--Scale Factors (2F10.0)

SCALV = scale factor for volumes. All volumes will be multiplied by this factor. (F10.0)

CONVV = conversion factor for volumes. (F10.0)

Record 3 is repeated NOSEG times:

Record 3--Segment Types and Volumes (3I10, 5F10.0)

ISEG = segment number.

IBOTSG = segment immediately below ISEG. (I10)

ITYPE(ISEG) = segment types: 1 = surface water segment, 2 = subsurface water segment, 3 = surface bed segment, 4 = subsurface bed segment, **5 = bottom bed segment**. (I10)

BVOL(ISEG) = volume of segment ISEG in cubic meters. (F10.0)

VMULT(ISEG) = hydraulic coefficient "a" for velocity in ISEG as a function of flow:

$$v = a Q^b$$

If b = 0, VMULT is a constant velocity in m/sec. (F10.0)

VEXP(ISEG) = hydraulic exponent "b" for velocity in ISEG as a function of flow (0-1). A value of 0.4 represents rectangular channels. (F10.0)

DMULT(ISEG) = hydraulic coefficient "c" for depth of ISEG as a function of flow:

$$d = c Q^d$$

If d = 0, DMULT is a constant depth in m. (F10.0)

DXP(ISEG) = hydraulic exponent "d" for depth of ISEG as a function of flow (0-1). A value of 0.6 represents rectangular channels. (F10.0)

Note that the four hydraulic geometry parameters are used to calculate segment velocity and depth, which are not used by WASP5 in transport calculations. These are used to calculate reaeration or volatilization from segments.

Records 1 and 2 are entered once for Data Group C. Record 3 is repeated NOSEG times. If ICFL = 2 in Data Group A, volumes are read from the restart file (*.RST, where * is the input data set name), and Records 2 and 3 should not be included in the input data set.

CHAPTER 5

DATA GROUP D: FLOWS

5.1 RECORD FORMATS

Data Group D provides for the advective transport flows that are used in the model. Flows may be input for up to 6 transport fields. Field one consists of advective flows in the water column. Field two consists of pore water flows. Fields three, four, and five consist of sediment transport velocities and cross-sectional areas for solids. A separate sediment transport field is specified for each of up to 3 solids types. Field six is for evaporation and precipitation velocities and cross-sectional areas. All flows may vary in time according to piecewise linear time functions.

Record 1 is read first. If IQOPT = 1 or 2, Data Block D1 is read next; if IQOPT = 3, Data Block D1 is skipped. Data Blocks D2, D3, D4, D5, and D6 follow in order for NFIELD = 2, 3, 4, 5, and 6, respectively. Following all specified Data Blocks, Record 32 is read.

Record 1--Data Input Options: Number of Flow Fields (2I5, A12)

IQOPT = flow option:

1 = field one (advective) flows are specified directly by user. Individual flows at each segment interface are summed by the model, and the net flow is applied across the interface.

2 = field one flows are specified directly by the user. Individual flows at each segment interface are applied directly by the model.

3 = flows are read from a formatted file created by DYNHYD5 or other hydrodynamic model. (I5)

4 = flows are read from an unformatted (or formatted) file created by GBHYDRO or other hydrodynamic model. (I5)

If option 1, 2, or 3 is chosen, complete this record and proceed to record 6.

NFIELD = number of flow fields. The first two fields are surface water and pore water flows. An additional field (3, 4, or 5) is used for each type of solid modeled. Field 6 is used for evaporation and precipitation. If no flows are used, set NFIELD to zero and continue with Data Group E. (I5)

IF IQOPT = 4, NFIELD must = 5

HYDFIL = name of hydrodynamic file to be read by WASP5 during the simulation (for example, RIVER1.HYD). (A12)

Record 2--External File Option: Field 1 flows (a40,i2,f10.0)

HYDROFIL = Name of File.

IRFILTYPE = File type; 0 = binary; 1= ASCII.

RWDTIME(2)= Time in days to rewind hydrodynamic file.

Currently, the user must make an entry for record 2 even if it is not to be used. To use the GBHYDRO external file as specified in record 2, set IQOPT = 4. To bypass, set IQOPT = 1, 2, or 3.

The required format for the flow dataset is as follows:

Initial read statements:

```
READ NOQS(1)                    !(Number of segment pairs)
READ (IR(I),JR(I),I=1,NOQS(1) !(I,J segment pairs)
READ TIME                       !(time in days)
```

IMPORTANT! GBTOXE expects TIME to be double precision.

Subsequent read statements:

Throughout the simulation, GBTOXE compares the current run time with the last time break read in. When the run-time exceeds the time break the next set of flows are read in along with the next time break. The format below should be repeated for the number of time breaks desired:

```
READ (qt(I),I=1,NOQS(1))        !(flows in m3/sec)
READ TIME                       !(time to next break)
```

Record 3--External File Option: Water Column Settling Velocities (a40,i2,f10.0)

GBSEDFIL1 = Name of File.

IRFILTYPE = File type; 0 = binary; 1= ASCII.

Currently, the user must make an entry for record 3 even if it not to be used. To bypass, set IQOPT = 1, 2, or 3. Note: GBTOXe does yet have the capability to rewind an external settling file.
The required format for the settling velocity dataset is as follows:

Initial read statements:

```
READ NOQS(1)                    !(Number of segment pairs)
READ (IR(I),JR(I),I=1,NOQS(1) !(I,J segment pairs)
READ TIME                       !(time in days)
```

IMPORTANT! GBTOXE expects TIME to be double precision.

Subsequent read statements:

Throughout the simulation, GBTOXE compares the current run time with the last time break read in. When the run-time exceeds the time break the next set of settling velocities are read in followed by the next time break. The format below should be repeated for the number of time breaks desired:

```
READ (qt(I),I=1,NOQS(1))        !(velocity in m/day)
READ TIME                       !(time to next break)
```

Record 4--External File Option: Water Column Deposition Velocities (a40,i2,f10.0)

GBSEDFIL2 = Name of File.

IDFILTYPE = File type; 0 = binary; 1= ASCII.

Currently, the user must make an entry for record 4 even if it not to be used.. To bypass, set IQOPT = 1, 2, or 3. Note: GBTOXe does yet have the capability to rewind an external deposition file.

The required format for the Deposition velocity dataset is as follows:

Initial read statements:

```
READ NOQS(1)                    !(Number of segment pairs)
READ (IR(I),JR(I),I=1,NOQS(1) !(I,J segment pairs)
READ TIME                       !(time in days)
```

IMPORTANT! GBTOXE expects TIME to be double precision.

Subsequent read statements:

Throughout the simulation, GBTOXE compares the current run time with the last time break read in. When the run time exceeds the time break the next set of settling velocities are read in followed by the next time break. The format below should be repeated for the number of time breaks desired:

```
READ (qt(I),I=1,NOQS(1))        !(velocity in m/day)
READ TIME                       !(time to next break)
```

Record 5--External File Option: Water Column Resuspension Velocities (a40,i2,f10.0)

GBSEDFIL3 = Name of File.

IUFILTYPE = File type; 0 = binary; 1= ASCII.

RWDTIME(3) = Time in days to rewind resuspension velocity file

Currently, the user must make an entry for record 5 even if it not to be used. To bypass, set IQOPT = 1, 2, or 3.

The required format for the resuspension velocity dataset is as follows:

Initial read statements:

```
READ NOQS(1)                    !(Number of segment pairs)
READ (IR(I),JR(I),I=1,NOQS(1) !(I,J segment pairs)
READ TIME                       !(time in days)
```

IMPORTANT! GBTOXE expects TIME to be double precision.

Subsequent read statements:

Throughout the simulation, GBTOXE compares the current run time with the last time break read in. When the run time exceeds the time break the next set of resuspension velocities are read in followed by the next time break. The format below should be repeated for the number of time breaks desired:

```
READ (qt(I),I=1,NOQS(1))      !(velocity in cm/day)
READ TIME                     !(time to next break)
```

Note: Resuspension velocities must have units of cm/day.

To use the external files as specified in records 3, 4, and 5 set NINQ(3) = -7; NINQ(4) = 0; NINQ(5) = 0. To bypass, follow specifications of DATA BLOCKS 1-6 as usual.

DATA BLOCK D1: Direct Input of Field One Flows (IQOPT = 1,2)

IF IQOPT = 4 skip DATA BLOCK D1 and proceed to DATA BLOCK D2

Record 6--Number of Flow Time Functions (I5, 2F10.0)

NINQ(1) = number of time functions for Field One. If no flows are used in field one, set NINQ to zero and skip to next field. (I5)

SCALQ = scaling factor. All flows in Field one are multiplied by SCALQ. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 3 – 6 are input as a group NINQ(1) times:

Record 7--Number of Flows (I5)

NOQS(1,NI) = number of unit flow responses in field one, time function NI; each unit flow is defined for a single segment pair. (I5)

Record 8--Flow Routing for Field One (4(F10.0, 2I15))

BQ(1,NI,K) = portion of flow for field one, time function NI that flows between segment pair K. (F10.0)

JQ(1,NI,K) = upstream segment. (I5)

IQ(1,NI,K) = downstream segment. (I5)

Record 4 is repeated NOQS(1,NI)/4 times.

Record 9--Number of Breaks in Advective Time Functions (I5)

NBRKQ(1,NI) = the number of flows and times used to describe piecewise linear time function NI. (I5)

Record 10--Piecewise Linear Advective Time Function (4(2F10.0))

QT(1,NI,K) = advective flow in m^3/s. (F10.0)

TQ(1,NI,K) = time in days. (F10.0)

Record 6 is repeated NBRKQ(1,NI) times.

Record 2 is input once for Data Block D1. Records 3, 4, 5, and 6 are input once for each flow time function. Record 4 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets per line. Record 6 uses as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D2: Field Two (Pore Water) Flows

Record 11--Number of Pore Water Time Functions (I5, 2F10.0)

NINQ(2) = number of pore water time functions. If no flows are used in Field Two, set NINQ to zero and skip to sediment transport fields. (I5)

SCALQ = scaling factor for pore water flows. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 8 – 11 are input as a group NINQ(2) times:

Record 12--Number of Flows (I5)

NOQS(2,NI) = number of segment pair flows in Field 2, time function NI. (I5)

Record 13--Flow Routing for Field Two (4(F10.0, 2I5))

BQ(2,NI,K) = portion of pore water flow for time function NI that flows between segment pair K. (F10.0)

JQ(2,NI,K) = upstream segment. (I5)

IQ(2,NI,K) = downstream segment. (I5)

Record 13 is repeated NOQS(2,NI)/4 times.

Record 14--Number of Breaks in Pore Water Time Function (I5)

NBRKQ(2,NI) = number of pore water flows and times used to describe piecewise linear time function NI. (I5)

Record 15--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(2,NI,K) = pore water flow in m^3/s. (F10.0)

TQ(2,NI,K) = time in days. (F10.0)

Record 15 is repeated NBRKQ(2,NI)/4 times.

Record 7 is input once for Data Group D2. Records 8, 9, 10 and 11 are input once for each pore water time function. Record 9 uses as many lines as necessary to input NOQS sets of BQ, JQ, and IQ, with four sets on each line. Record 11 uses as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D3: Sediment 1 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids are modeled, skip directly to Record ? (Flow Bypass Options).

Record 16--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(3) = number of velocity time functions for Field 3. (I5)

IF IQOPT = 4, NINQ(3) Must = -7. Complete this record and proceed to record 21

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 17 – 20 are input as a group NINQ(3) times:

Record 17--Number of Segment Pairs (I5)

NOQS(3,NI) = number of segment pairs involved in sediment 1 transport. (I5)

Record 18--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(3,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(3,NI,K) = segment sediment is transported from. (I5)

IQ(3,NI,K) = segment sediment is transported to. (I5)

Record 18 is repeated NOQS(3,NI)/4 times.

Record 19--Number of Breaks in Velocity Time Function (I5)

NBRKQ(3,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 20--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(3,NI,K) = sediment 1 transport velocity in m/s. (F10.0)

TQ(3,NI,K) = time in days. (F10.0)

Record 20 is repeated NBRKQ(3,NI)/4 times.

Record 16 is input once for Data Block D3. Records 17, 18, 19 and 20 are input for each velocity time function. Record 18 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 16 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D4: Sediment 2 Transport Field

Sediment transport flow data are input as velocities and

areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 2 are modeled, enter 0 for NINQ(4), then skip directly to the next data block.

Record 21--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(4) = number of velocity time functions for Field 4. (I5)

IF IQOPT = 4, NINQ(4) Must = 0. Complete this record and proceed to record 26

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 22 – 25 are input as a group NINQ(4) times:

Record 22--Number of Segment Pairs (I5)

NOQS(4,NI) = number of segment pairs involved in sediment 2 transport. (I5)

Record 23--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(4,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(4,NI,K) = segment sediment is transported from. (I5)

IQ(4,NI,K) = segment sediment is transported to. (I5)

Record 23 is repeated NOQS(4,NI)/4 times.

Record 24--Number of Breaks in Velocity Time Function (I5)

NBRKQ(4,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 25--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(4,NI,K) = sediment 2 transport velocity in m/s. (F10.0)

TQ(4,NI,K) = time in days. (F10.0)

Record 25 is repeated NBRKQ(4,NI)/4 times.

Record 21 is input once for Data Block D4. Records 22, 23, 24 and 25 are input for each velocity time function. Record 23 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 25 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D.5: Sediment 3 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 3 are modeled, enter 0 for NINQ(5), then skip directly to the next data block.

Record 26--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(5) = number of velocity time functions for Field 5. (I5)

IF IQOPT = 4, NINQ(5) Must = 0. Complete this record and proceed to record 31

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 27 – 30 are input as a group NINQ(5) times:

Record 27--Number of Segment Pairs (I5)

NOQS(5,NI) = number of segment pairs involved in sediment 3 transport. (I5)

Record 28--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(5,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(5,NI,K) = segment sediment is transported from. (I5)

IQ(5,NI,K) = segment sediment is transported to. (I5)

Record 28 is repeated NOQS(5,NI)/4 times.

Record 29--Number of Breaks in Velocity Time Function (I5)

NBRKQ(5,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 30--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(5,NI,K) = sediment 3 transport velocity in m/s. (F10.0)

TQ(5,NI,K) = time in days. (F10.0)

Record 30 is repeated NBRKQ(5,NI)/4 times.

Record 26 is input once for Data Block D5. Records 27, 28, 29 and 30 are input for each velocity time function. Record 28 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 30 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D6: Evaporation and Precipitation Field

Evaporation and precipitation flow data are input as velocities and areas. Velocities may vary in time to represent rainfall events or seasonal evaporation. No chemical is transported with evaporation, but volumes are adjusted to maintain continuity. If this field is not modeled, skip directly to Record 32 (Flow Bypass Options). After all transport field data are entered, Record 32 is input with NOSYS entries. If no evaporation or precipitation fields are specified, Record 32 follows Data Group D.5 (solids 3 transport).

Record 31--Number of Velocity Time Functions (I5, 2F10.0))

NINQ(6) = number of velocity time functions for Field 6. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 32 – 35 are input as a group NINQ(6) times:

Record 32--Number of Segment Pairs (I5)

NOQS(6,NI) = number of segment pairs involved in evaporation or precipitation. (I5)

Record 33--Areas for Evaporation, Precipitation (4(F10.0, 2I5))

BQ(6,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(6,NI,K) = segment water is transported from; if = 0, this is precipitation. (I5)

IQ(6,NI,K) = segment water is transported to; if = 0, this is evaporation. (I5)

Record 33 is repeated NOQS(6,NI)/4 times.

Record 34--Number of Breaks in Velocity Time Function (I5)

NBRKQ(6,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 35--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(6,NI,K) = water transport velocity in m/s; if more traditional units of cm/day or cm/year are desired, then specify CONVQ = $1.1574E^{-7}$ or $3.169E^{-10}$, respectively. (F10.0)

TQ(6,NI,K) = time in days. (F10.0)

Record 35 is repeated NBRKQ(6,NI)/4 times.

END OF DATA BLOCKS FOR D

CHAPTER 6

DATA GROUP E: BOUNDARY CONCENTRATIONS

Data Group E supplies concentrations for each system at the model network boundaries. Model boundaries consist of those segments that import, export, or exchange water with locations outside the network, as specified in Data Groups B and D. All system concentrations from 1 to NOSEG must be supplied for each boundary. Boundary concentrations vary with time following a piecewise linear time function specified by the user in Records 3 and 4.

6.1 RECORD FORMATS

Data Group E is repeated, in its entirety, NOSYS times.

Record 1--Data Input Option--Number of Boundary Conditions (I10, 70X)

NOBC(K) = number of boundary conditions used for system K. (I10)

TITLE = name of data group. (70X)

If no boundary conditions are to be input for system K, set NOBC(K) equal to zero and either continue with the next system or go to Data Group F if K is the last system.

Record 2--Scale Factor for Boundary Conditions (2F10.0)

SCALB = scale factor for boundary conditions. All boundary conditions will be multiplied by this factor. (F10.0)

CONVB = unit conversion factor for boundary conditions. Boundary conditions are expected to be in mg/L (i.e. - g/m^3), in which case CONVB will be 1.0. (F10.0)

Records 3-4 are input as a unit NOBC(K) times:

Record 3--Boundary Location (2I5)

IBC(K) = boundary segment number. (I5)

NOBRK(K) = number of values and times used to describe the broken line approximation. The number of breaks must be equal for all boundary conditions within a system. (I5)

Record 4--Boundary Concentrations (4(2F10.0))

BCT(K) = value of the boundary concentration at time T(K) in mg/L. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the broken line approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic, with period equation to T(NOBRK). All break times must agree for all segments, i.e., T(1) must be the same for all boundaries, T(2) must be the same for all boundaries, etc. (F10.0)

Record 4 is repeated NOBRK(K)/4 times.

Records 1 and 2 are entered once. Records 3 and 4 are a set and are repeated NOBC times. Within each NOBC set, Record 3 is entered once and Record 4 is repeated until NOBRK entries are input. Four entries (four BCT(K)-T(K) pairs) will fit on each 80-space line. The whole group (Records 1 - 4) is repeated NOSYS times, once for each model system.

Data Group E is input NOSYS times, once for each system simulated. NOSYS is specified in Data Group A, and has a maximum value of 6. For those systems being bypassed, the user may specify 0 for the number of boundary conditions, and skip to the next system.

The user should be careful to note that all boundary concentrations are input in units of mg/L (even though the output concentrations for chemical are in units of ng/L.)

CHAPTER 7

DATA GROUP F: WASTE LOADS

Data Group F is composed of two blocks of data. Data Block F1 contains the point source waste loads used in the model. These loads vary with time following a piecewise linear time function specified by the user in Records 3 and 4. Following complete specification of point source loads, nonpoint source loads are read from Data Block F2, which is composed of only one record in the input dataset. Nonpoint source loads vary with time in a daily step function read from an external loading file.

7.1 RECORD FORMATS

Data Block F1 (records 1-4) is repeated in its entirety NOSYS times:

Record 1--Number of Point Source Loadings (I10, 70X)

NOWK(ISYS) = number of point source loadings used for system ISYS. Loadings may also be considered as sources (loads) or sinks of a water quality constituent. If no loadings are to be input, set NOWK(ISYS) to zero, and continue with next system or go to next data group.(I10)

TITLE = name of data group. (70X)

If no point source loadings are to be input for system ISYS, set NOWK(ISYS) equal to zero and either continue with the next system or go to Data Group G if ISYS is the last system.

Record 2--Scale Factor for Point Source Loadings (2F10.0)

SCALW = scale factor for point source loadings. All loadings for system ISYS will be multiplied by this factor. (F10.0)

CONVW = unit conversion factor for point source loadings for system ISYS. Loadings are expected to be in kilograms per day. If loadings are given in English units (pounds per day), this factor will be 0.4535. (F10.0)

Records 3-4 are input as a unit NOWK(ISYS) times:

Record 3--Number of Point Sources (2I5)

IWK(K) = segment number that has point source loading BWK(K). (I5)

NOBRK(K) = number of breaks used to describe the loading function approximation. The number of breaks must be equal for all forcing functions within a system. (I5)

Record 4--Point Source Time Function (4(2F10.0))

WKT(K) = value of the point source loading at time T(K), in kg/day. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic with period equal to T(NOBRK). All break times must agree for all segments; i.e., T(1) must be the same for all loads, T(2) must be the same for all loads, etc. (F10.0)

Record 4 is repeated NOBRK(ISYS)/4 times.

Records 1 and 2 are input once. Records 3 and 4 are a set and are repeated (as a set) NOWK times. Within each set, Record 3 is entered once and Record 4 is repeated until all NOBRK entries are entered. Four entries (WKT(K)-T(K) pairs) will fit on each 80-space line. The entire group (Records 1 - 4) is repeated NOSYS times, once for each system.

Data Block F2, record 5, is input once:

Record 5--Nonpoint Source Load Option (I10)

LOPT = nonpoint source load option; a value of 0 means that no nonpoint sources will be read from an external file; a value of 1 will cause the model to read a set of loads from an external file. The user will be prompted by WASP5 to provide information on the external file. This file and its contents are described below. (I10)

7.2 THE EXTERNAL NONPOINT SOURCE FILE

When LOPT is set to 1, external nonpoint sources will be read from a formatted ASCII file chosen by the user. This file contains information on which WASP5 systems and segments receive nonpoint source loads, and a record of the nonzero loads by system, segment, and day.

Six records comprise the nonpoint source file.

Record 1--Data Options (A15, 3I5)

NPSMOD	=	Name or description of nonpoint source model or method of generation; this is echoed to the output file for the record. (A15)
NUMSEG	=	Number of segments receiving nonpoint source loads. (I5)
INTOPT	=	Interpolation option; 1 = step function (only one in code now). (I5)
NUMSYS	=	Number of WASP systems receiving nonpoint source loads. (I5)

Record 2--Loading Segments (I5)

LSEG(I)	=	segment number receiving loads. (I5)

Record 2 is repeated NUMSEG times.

Record 3--Loading Systems (20I5)

LSYS(I)	=	WASP system numbers receiving loads. (I5)

Record 4--System Descriptors (A15)

NAMESY(I)	=	Name or description of WASP systems receiving loads. (A15)

Record 4 is repeated NUMSYS times.

Records 5 and 6 are repeated as a unit for the number of days that nonzero loads occur:

Record 5--Loading Days (F10.0)

LDAY = Time in days for the following nonzero load. (F10.0)

Record 6--Nonpoint Source Loads (A15, 20F10.0)

NAMESY(I) = System name or description (not read in by WASP). (A15)

NPSWK(I,J) = Nonpoint source loads for WASP system "I" at all loading segments "J", in the order presented in Record 2. Loads are in kg/day. (20F10.0)

Record 6 is repeated NUMSYS times.

Record 1 is input once. Record 2 is repeated NUMSEG times. Record 3 is then input once. Record 4 is repeated NUMSYS times. Records 5 and 6 are a set and are repeated (as a set) NUMSYS times. Within each set, Record 5 is entered once and Record 6 is repeated NUMSYS times.

Data Block F1 is input NOSYS times, once for each system simulated. NOSYS is specified in Data Group A, and has a maximum value of 6. For those systems being bypassed, the user may specify 0 for the number of waste loads, and skip to the next system.

CHAPTER 8

DATA GROUP G: PARAMETERS

Parameters are spatially-variable characteristics of the water body. The definition of the parameters will vary, depending upon the structure and kinetics of the systems comprising each model. The input format, however, is constant. The number of parameters that is specified in Record 1 must be input for each segment.

8.1 RECORD FORMATS

Record 1--Number of Parameters (I10, 70X)

NOPAM	=	number of parameters required by the model. If no parameters are to be input, set NOPAM to zero and go to Data Group H. (I10)
TITLE	=	name of data group. (70X)

Record 2--Scale Factors for Parameters (4(A5, I5, F10.0))

ANAME(ISC)	=	descriptive name for parameter ISC. (A5)
ISC	=	parameter number identifying parameter. (I5)
PSCAL(ISC)	=	scale factor for parameter ISC. (F10.0)

Record 2 is repeated NOPAM/4 times.

Records 3-4 are input as a unit NOSEG times:

Record 3--Segment Number (I10)

ISG	=	segment number for the following parameter values. (I10)

Record 4--Segment Parameters (4(A5, I5, F10.0))

PNAME(ISC)	=	an optional one to five alphanumeric character descriptive name for parameter PARAM(ISG,ISC). (A5)
ISC	=	parameter number identifying parameter. (I5)
PARAM(ISEG,ISC)	=	the value of parameter ISC in segment ISG. (F10.0)

Record 4 is repeated NOPAM/4 times.

Record 1 is input once in Data Group G, occupying one line. Record 2 has NOPAM entries. Four entries will fit on one line; thus, Record 2 uses as many 80-space lines as needed to enter all NOPAM entries. Records 3 and 4 are repeated NOSEG times, once for each segment. For each segment, Record 4 uses as many lines as needed to enter all NOPAM entries.

Listed below are the 26 parameters that may be used by GBTOXe. The user need input only those required to model the particular reactions being considered.

ISC	ANAME	Definition, Units, and Reactions Affected
1	VELFN	Pointer to water velocity time function (1-4); V.
2	TMPFN	Pointer to normalized temperature time function (1-4); ALL.
3	TEMP	Multiplier for water temperature time function (EC); ALL.
4	WVEL	Multiplier for wind velocity (10 meters above segment surface) time function (meters/sec); V.
5	REAR	Multiplier of time function 5, whose definition depends on volatilization option XV (constants 236,736,1336): XV = 1 volatilization rate constant (m/day) XV = 2,3 oxygen reaeration rate constant (m/day) XV = 4,5 REAER not used; enter 0; V.
6	DOC	Dissolved organic carbon concentrations (mg/L); S, P.
7	FOC 1	Fraction organic carbon of solids class 1; S.
8	FOC 2	Fraction organic carbon of solids class 2; S.
9	FOC 3	Fraction organic carbon of solids class 3; S.
10	CHPHL	Multiplier for phytoplankton chlorophyll concentration time function (mg/L); P.
11	PH	Multiplier for pH time function; H, I.
12	XKE2	Light extinction coefficient for photochemically

ISC	ANAME	Definition, Units, and Reactions Affected
		active light (1/meter); this value is used only for photolysis option XPHOTO = 2 (constants 286,886,1486). For photolysis option 1 or 2 when XKE2 = 0.0 the extinction coefficient is calculated from solids, DOC, and chlorophyll concentrations; P.
13	OXRAD	Concentration of oxidants, such as O_3 for H_2O_2 (moles/L); O.
14	BAC	Density of active bacteria (cells/100 cc) the units for bacterial density must be consistent with those used for the second order biodegradation rate constants KBIO20 (constants 146-160, 746-760, 1346-1360); the product of BAC and KBIO20 must be units of day^{-1}; B.
15	EXENV	Property of aquatic environment that affects the user-defined "extra reaction." The units for EXENV must be consistent with those used for second order rate constants KE20 (constant 576-590, 1176-1190, 1776-1790); the product of EXENV and KE20 must yield units of day^{-1}; E.
16	TOTKG 1	Total lumped first-order decay rate constant for chemical 1 in segment (day^{-1}).
17	TOTKG 2	Total lumped first-order decay rate constant for chemical 2 in segment (day^{-1}).
18	TOTKG 3	Total lumped first-order decay rate for chemical 3 in segment (day^{-1}).
19	**KDIF1**	**Chemical 1 pore water diffusion coefficient multiplier**
20	**KDIF2**	**Chemical 2 pore water diffusion coefficient multiplier**
21	**KDIF3**	**Chemical 3 pore water diffusion coefficient multiplier**
22	**KDIF4**	**Solids 1 pore water diffusion coefficient multiplier**
23	**KDIF5**	**Solids 2 pore water diffusion coefficient multiplier**
24	**KDIF6**	**Solids 3 pore water diffusion coefficient multiplier**

ISC	ANAME	Definition, Units, and Reactions Affected
25	**KDIF7**	**Solids 4 pore water diffusion coefficient multiplier**
26	**PORR**	**Fraction water**

I = ionization, S = sorption, V = volatilization, B = biodegradation, H = hydrolysis, O = oxidation, P = photolysis, E = extra reaction

CHAPTER 9

DATA GROUP H: CONSTANTS

The definition of the constants will vary, depending upon the structure and kinetics of the systems comprising each model. This data group is subdivided into global constants and constants for each system (thus NOSYS+1 groups are read). Each of these groups can be subdivided into any number of fields containing similar kinds of data.

9.1 RECORD FORMATS

Record 1--Header (80X)

TITLE = name of data group. (80X)

Records 2-4 are input as a group NOSYS+1 times:

Record 2--Data Fields in Group ISYS (A10, I10)

CHNAME(ISYS) = a ten-character descriptive name for System (ISYS). (A10)

NFLD = number of fields of constants for this group; 0 = no constants for this group; the user may subdivide the constants into any number of arbitrary fields. (I10)

If no constants are to be input for this group, set NFLD equal to zero and continue with next group. Records 3 and 4 are repeated as a unit NFLD times.

Record 3--Number of Constants in Field (A10, I10)

FLDNAME = ten-character name identifying field of constants. (A10)

NCONS = number of constants to be entered in this field; 0 = no constants for this field (skip to next field). (I10)

Record 4--Constants (2(A10, I10, F10.0))

TNAME(ISC) = name identifying constant ISC. (A10)

ISC = number identifying constant; these numbers are set by model developer. (I10)

CONST(ISC) = value of constant ISC. (F10.0)

Record 4 is repeated NCONS/2 times.

Record 1 is entered once in Data Group H. Records 2 through 4 are entered as NOSYS + 1 groups. For each group, Records 3 and 4 are entered NFLD times. For each field, Record 4 uses as many lines as needed for NCONS entries (2 per line).

In WASP5, a large number of constants are available to characterize the various chemical reactions at different levels of complexity. The constants applicable to GBTOXe are summarized in the tables below. The tables include the additional constants added in the development of GBTOX and the pertinent WASP5 constants.

TABLE 1 CONSTANTS FOR SIMPLE TOXI4 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
111	711	1311	PIXC(1,1)	Constant partition coefficient for sorption to solids (class 1), l_w/kgs
			K_i:	First order loss rate constants, day^{-1}
140	740	1340	KV	Volatilization
141	741	1341	KBW	Water column biodegradation
142	742	1342	KBS	Benthic biodegradation
181	781	1381	KHOH	Alkaline hydrolysis
182	782	1382	KHN	Neutral hydrolysis
183	783	1383	KHH	Acid hydrolysis
256	856	1456	KO	Oxidation
287	887	1487	KF	Photolysis
571	1171	1771	KE	Extra reaction
			TH_i	Half lives for reactions, day
143	743	1343	THBW	Water column biodegradation
144	744	1344	THBS	Benthic biodegradation
252	852	1452	THHOH	Alkaline hydrolysis
253	853	1453	THHN	Neutral hydrolysis
254	854	1454	THHH	Acid hydrolysis
257	857	1457	THO	Oxidation
289	889	1489	THF	Photolysis
572	1172	1772	THE	Extra reaction

TABLE 2 GENERAL CHEMICAL CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
9	609	1209	TDINT	Time interval at which rate constants are recomputed, days
81	681	1281	MOLWT	Molecular weight, g/mole
82	682	1282	SOLG	Solubility, mg/L
83	683	1283	VAPRG	Vapor pressure, torr
84	684	1284	LKOW	Log octanol-water partition coefficient, L_o/L_w

TABLE 3 VOLATILIZATION CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
136	736	1336	XV	Volatilization option: 0 = no volatilization 1 = measured volatilization 2 = measured reaeration + O'Conner for gas transfer 3 = measured reaeration + MacKay for gas transfer 4 = calculated using O'Conner 5 = calculated using MacKay
137	737	1337	HENRY	Henry's constant, atm-m^3/mole
138	738	1338	KLT	Volatilization temperature correction factor, dimensionless
139	739	1339	KVOG	Measured ratio of volatilization to reaeration rates
2	2	2	WTYPE	Water body type (0 = flowing stream, river, or estuary; 1 = stagnant pond or lake)
5	5	5	AIRTMP	Multiplier for air temperature time function
8	608	1208	ATMOS	Atmospheric concentration of chemical, Fg/L

TABLE 4 GBTOX/GBTOXe CHEMICAL CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
2301	2401	2501	K9WDIS	User defined first-order transformation rate of dissolved chemical in water column
2302	2402	2502	K9WDOC	User defined first-order transformation rate of DOC in water column
2303	2403	2503	K9WBIC	User defined first-order transformation rate of BIC in water column
2304	2404	2504	K9WPDC	User defined first-order transformation rate of PDC in water column
2305	2405	2505	K9WS4	User defined first-order transformation rate of ? in water column
2321	2421	2521	K9BDIS	User defined first-order transformation rate of dissolved chemical in sediment
2322	2422	2522	K9BDOC	User defined first-order transformation rate of DOC in sediment
2323	2423	2523	K9BBIC	User defined first-order transformation rate of BIC in sediment
2324	2424	2524	K9BPDC	User defined first-order transformation rate of PDC in sediment
2325	2425	2525	K9BS4	User defined first-order transformation rate of ? in sediment
2311	2411	2511	T9WDIS	Temperature correction coefficient for K9WDIS
2312	2412	2512	T9WDOC	Temperature correction coefficient for K9WDOC

TABLE 4 GBTOX/GBTOXe CHEMICAL CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
2313	2413	2513	T9WBIC	Temperature correction coefficient for K9WBIC
2314	2414	2514	T9WPDC	Temperature correction coefficient for K9WPDC
2315	2415	2515	T9WS4	Temperature correction coefficient for K9WS4
2331	2431	2531	T9BDIS	Temperature correction coefficient for K9BDIS
2332	2432	2532	T9BDOC	Temperature correction coefficient for K9BDOC
2333	2433	2533	T9BBIC	Temperature correction coefficient for K9BBIC
2334	2434	2534	T9BPDC	Temperature correction coefficient for K9BPDC
2335	2435	2535	T9BS4	Temperature correction coefficient for K9BS4

TABLE 5 GBTOX/GBTOXe SOLIDS CONSTANTS

Constant Number	Variable	Definition
2112	YIELD12	Yield coefficient applied to transformation of solids 1 to solids 2
2113	YIELD13	Yield coefficient applied to transformation of solids 1 to solids 3
2114	YIELD14	Yield coefficient applied to transformation of solids 1 to solids 4
2121	YIELD21	Yield coefficient applied to transformation of solids 2 to solids 1
2123	YIELD23	Yield coefficient applied to transformation of solids 2 to solids 3
2124	YIELD24	Yield coefficient applied to transformation of solids 2 to solids 4
2131	YIELD31	Yield coefficient applied to transformation of solids 3 to solids 1
2132	YIELD32	Yield coefficient applied to transformation of solids 3 to solids 2
2134	YIELD34	Yield coefficient applied to transformation of solids 3 to solids 4
2141	YIELD41	Yield coefficient applied to transformation of solids 4 to solids 1
2142	YIELD42	Yield coefficient applied to transformation of solids 4 to solids 2
2143	YIELD43	Yield coefficient applied to transformation of solids 4 to solids 3

TABLE 5 GBTOX/GBTOXe SOLIDS CONSTANTS

Constant Number	Variable	Definition
2212	YSOLFR12	Fraction Solids 1 applied to transformation of solids 1 to solids 2
2213	YSOLFR13	Fraction Solids 1 applied to transformation of solids 1 to solids 3
2214	YSOLFR14	Fraction Solids 1 applied to transformation of solids 1 to solids 4
2221	YSOLFR21	Fraction Solids 2 applied to transformation of solids 2 to solids 1
2223	YSOLFR23	Fraction Solids 2 applied to transformation of solids 2 to solids 3
2224	YSOLFR24	Fraction Solids 2 applied to transformation of solids 2 to solids 4
2231	YSOLFR31	Fraction Solids 3 applied to transformation of solids 3 to solids 1
2232	YSOLFR32	Fraction Solids 3 applied to transformation of solids 3 to solids 2
2234	YSOLFR34	Fraction Solids 3 applied to transformation of solids 3 to solids 4
2241	YSOLFR41	Fraction Solids 4 applied to transformation of solids 4 to solids 1
2242	YSOLFR42	Fraction Solids 4 applied to transformation of solids 4 to solids 2
2243	YSOLFR43	Fraction Solids 4 applied to transformation of solids 4 to solids 3

TABLE 5 GBTOX/GBTOXe SOLIDS CONSTANTS

Constant Number	Variable	Definition
2001	KSW1	User defined first-order degradation rate for solids fraction 1 in water column($days^{-1}$)
2002	KSW2	User defined first-order degradation rate for solids fraction 2 in water column($days^{-1}$)
2003	KSW3	User defined first-order degradation rate for solids fraction 3 in water column($days^{-1}$)
2004	KSW4	User defined first-order degradation rate for solids fraction 4 in water column($days^{-1}$)
2011	KSB1	User defined first-order degradation rate for solids fraction 1 in sediments($days^{-1}$)
2012	KSB2	User defined first-order degradation rate for solids fraction 2 in sediments ($days^{-1}$)
2013	KSB3	User defined first-order degradation rate for solids fraction 3 in sediments ($days^{-1}$)
2014	KSB4	User defined first-order degradation rate for solids fraction 4 in sediments ($days^{-1}$)
2005	THW1	Temperature correction coefficient for KSW1
2006	THW2	Temperature correction coefficient for KSW2
2007	THW3	Temperature correction coefficient for KSW3
2008	THW4	Temperature correction coefficient for KSW4
2015	THS1	Temperature correction coefficient for KSB1
2016	THS2	Temperature correction coefficient for KSB2

TABLE 5 GBTOX/GBTOXe SOLIDS CONSTANTS

Constant Number	Variable	Definition
2017	THS3	Temperature correction coefficient for KSB3
2018	THS4	Temperature correction coefficient for KSB4
2051	KMS1	Michaelis half saturation constant for solids fraction 1 degradation in water column
2052	KMS2	Michaelis half saturation constant for solids fraction 2 degradation in water column
2053	KMS3	Michaelis half saturation constant for solids fraction 3 degradation in water column
2054	KMS4	Michaelis half saturation constant for solids fraction 4 degradation in water column

CHAPTER 10

DATA GROUP I: KINETIC TIME FUNCTIONS

The definition of the kinetic time functions will vary depending upon the structure and the kinetics of the systems comprising each model. The input format, however, is constant. Time functions are input as piecewise linear functions.

10.1 RECORD FORMATS

Record 1--Number of Time Functions (I10, 70X)

NFUNC	=	number of time functions required by the model. If no time functions are to be input, set NFUNC equal to zero and go to Data Group J. (I10)
TITLE	=	name of data group. (70X)

Records 2-3 are input as a group NFUNC times:

Record 2--Time Function Descriptions (A5, 2I5)

ANAME(ISC)	=	an optional one to five alphanumeric character descriptive name for the time function I. (A5)
NOBRK(ISC)	=	number of breaks used to describe the time function I. (I5)
ISC	=	number identifying the time function; these numbers are set by the model developer. (I5)

Record 3--Time Functions (4(2F10.0))

VALT(K)	=	value of time function ISC at time T(K). (F10.0)
T(K)	=	time in days. If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to be periodic, with period equal to T(NOBRK). (F10.0)

Record 3 is repeated NOBRK(ISC)/4 times.

Record 1 in entered once in Data Group I. Records 2 and 3, as a set, are repeated NFUNC times. Within each NFUNC set, Record 2 is input once and Record 3 uses as many 80-space lines as needed to input NOBRK entries. Four entries (four VALK(K)-T(K) pairs) will fit on each 80-space line.

10.2 THE TOXIC CHEMICAL MODEL

Listed below are the 17 time functions available in TOXI4. The parameters and time functions interact in such away to allow the user segment specific control of environmental data. For more details see the parameter input section.

Two of the time functions operate in conjuction with a parameter "pointer" in Data Group G. The parameter value specifies which of four time functions for temperature or water velocity are to be associated with each segment. Time functions 1-4 are the four temperature functions available for parameter TMPFN. Time functions 5-8 are the four water velocity options for VELFN.

ISC	ANAME	VALT(ISC)
1	TEMPN(1)	Time-variable temperature function 1. TEMPN(K) can be either a normalized function or an actual temperature in EC, depending upon the definition of the parameter multiplier TEMP(ISEG).
2	TEMPN(2)	Time variable temperature function 2, unitless or EC.
3	TEMPN(3)	Time variable temperature 3, unitless or EC.
4	TEMPN(4)	Time variable temperature 4, unitless or EC.
5	**TEMPN(5)**	**Time variable temperature 5, unitless or EC.**
6	**TEMPN(6)**	**Time variable temperature 6, unitless or EC.**
7	**TEMPN(7)**	**Time variable temperature 7, unitless or EC.**
8	VELN(1)	Time variable velocity function 1, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C.

9	WINDN	Time variable wind function, m/sec. This time function is multiplied by the segment specific wind multiplier WVEL entered in the parameter section.
10	PHNW	Time variable ph function. This time function is multiplied by the segment specific ph multiplier ph enter in the parameter section.
11	PHNS	Normalized benthic pH function, dimensionless. This is multiplied by the segment pH multiplier PH(ISEG) for benthic segments.
12	REARN	Time variable reaeration coefficient, per day. This variable is multiplied by the segment specific variable REAR. entered in the parameter section.
13	AIRTMPN	Air temperature, C. Used for calculating reaeration rate.
14	CHLN	Phytoplankton chlorophyll concentration, mg/l. This variable is multiplied by the segment specific variable CHPHL entered in the parameter section
15	PHTON	Normalized light intensity, dimensionless. This is used for photolysis option 2 to adjust the measured rate constant under controlled light intensity to a predicted rate constant under ambient light intensity.
16	BACNW	Time variable bacteria concentration in the water column, mg/l. This is multiplied by the segment specific multiplier BAC entered in the parameter section.
17	BACNS	Normalized benthic bacteria function, dimensionless. This is multiplied by the segment bacteria multiplier BAC(ISEG) for benthic segments.
261	**ATMC1**	**Chemical 1 atmospheric concentration ug/L.**
262	**ATMC2**	**Chemical 2 atmospheric concentration ug/L.**
263	**ATMC3**	**Chemical 3 atmospheric concentration ug/L.**

TEMPN can affect all reactions. Volatilization option 1 uses REARN. Volatilization options 4 and 5 use WINDN and AIRTMPN. Volatilization options 2 and 3 use either VELN or REARN. Functions not specified default to 1.0.

CHAPTER 11

DATA GROUP J: INITIAL CONDITIONS

11.1 RECORD FORMATS

The initial conditions are the segment concentrations and densities for the state variables at time zero (the start of the simulation).

Records 1-2 are input as a group NOSYS times:

Record 1--System Information (A40, I5, F5.0, F10.0, 20X)

CHEML	=	chemical or system name (A40).
IFIELD	=	solids field (3, 4, or 5) that transports this system in its pure or sorbed form (I5).
DSED	=	density of system; 0.0 for chemical, 0.5-2.5 for solids, kg/L. (F5.0).
CMAX	=	maximum concentration allowed, mg/L. (F10.0)
TITLE	=	name of data group. (20X)

Record 2--Initial Conditions (3(A5, 2F10.0))

ANAME(K)	=	an optional one to five alphanumeric character descriptive name or number identifying segment K. (A5)
C(ISYS,K)	=	initial concentration in segment K of system ISYS in the appropriate units, mg/L. (F10.0)
DISSF	=	dissolved fraction of chemical in segment K. (F10.0)

Record 2 is repeated NOSEG/3 times.

Records 1 and 2 are a set and will be repeated NOSYS times. Within each NOSYS set, Record 2 will use as many 80-space lines as needed to input NOSEG entries. Three entries (ANAME-C-DISSF) will fit on one line. After NOSEG entries have been entered in a NOSYS set, begin the next NOSYS set on the following line. If ICFL = 2 in Data Group A, initial conditions are read from the restart file (*.RST, where * is the input data set name), and

Data Group J should not be included in the input data set.

Data Group J is input as a unit NOSYS times, once for each system. In record 1, solids transport fields must be specified for each solid (i.e.- variables 4, 5, 6, and 7). While solids transport fields are also specified for each chemical (variables 1, 2, and 3), the values are nominal. GBTOXe will calculate the actual transport of the sorbed chemical fractions using internal partitioning relationships.

In Record 2, the dissolved fraction of each system in each segment must be specified. These values should be 1.0 for each solid variable (4, 5, 6, and 7). Dissolved fraction values for each chemical are nominal. GBTOXe will calculate the actual dissolved fractions using internal partitioning relationships.

CHAPTER 12

GBTOXe OUTPUT

12.1 GENERAL CONSIDERATIONS

GBTOXe simulations produce several files that may be examined by the user. These files use the file name of the input data set with a unique extension.

Other files created by GBTOXe include *.OUT, *.MSB, and restart.out (where * is the name of the input data set). The *.OUT file contains a record of the input data plus any simulation error messages that may have been generated.

The TRN file contains a set of transport-associated variables for each segment at each print interval throughout the simulation. These variables include the time step (day), calculated maximum time steps (day), segment volumes (m^3), segment flows (m^3/sec), flow changes (m^3/sec), time constants for segment flow (day^{-1}), segment exchange flows (m^3/sec), the time constant for segment exchanges (day^{-1}), the segment dispersion coefficient (m^3/sec), and the numerical dispersion coefficient (m^2/sec).

The MSB file contains a mass balance record for one designated system in the model network as a whole (in kg). For each print interval, this file records the accumulated mass in from advection, dispersion, and loading; the accumulated mass out through advection, dispersion, burial (or volatilization, and kinetic transformation; the total resident mass; and the residual (unaccounted for) mass.

The restart.out file contains a snapshot of volumes and concentrations of each system in each segment at the conclusion of the simulation. This file can be read by GBTOXe to continue a series of simulations.

GBTOXe generates two groups of output files. The first group represents output of instantaneous results for each model segment for the duration of the simulation at time intervals specified in the input file. Seven of these files are generated, one for each state variable. They are given the same name as the input file and are suffixed with a “.dm” followed by the number corresponding to the system number (same as WASP). The output files start with a header that describes the information it contains. However, for the current version of GBTOXe, only the

concentration information (volume and carbon based) should be considered valid output.

The second group represents the spatially and temporally averaged chemical concentration results. The spatial and temporal extent of averaging is specified in Data Group A. Currently this feature is only implemented for the chemical 1 state variable. GBTOXe creates two files that contain the averaged results for the "zones" specified in Data Group A. Averaged results are output in a sequential, columned format. A description of each field is presented in the table below. Gbtoxe2.avg was created to provide a depth weighted average of organic carbon normalized chemical concentrations in the sediments of thickness 0-5 cm and 0-10 cm. The water column information in these files are identical but it should be noted that 1) gbtoxe2.avg does not have a biotic carbon normalized chemical concentration field and 2) the units of the dissolved chemical concentration field in gbtoxe2.avg are μg/L.

File Name	Column Range	Field Description
Gbtoxe1.avg	1-12	Time (Days)
	32-24	Zone Label
	25-39	Average Water column dissolved chemical concentration (ng/L)
	40-54	Average Water column organic carbon normalized chemical concentration (ug/gOC)
	55-69	Average Water column biotic carbon normalized chemical concentration (ug/gOC)
	70-84	Average Sediment organic carbon normalized chemical concentration 0-2 cm (ug/gOC)
	85-99	Average Sediment organic carbon normalized chemical concentration 2-4 cm (ug/gOC)

	100-114	Average Sediment organic carbon normalized chemical concentration 4-10 cm (ug/gOC)
Gbtoxe2.avg	1-12	Time (Days)
	32-24	Zone Label
	25-39	Average Water column dissolved chemical concentration (μg/L)
	40-54	Average Water column biotic carbon normalized chemical concentration (ug/gOC)
	55-69	Average Sediment organic carbon normalized chemical concentration 0-5 cm (ug/gOC)
	70-84	Average Sediment organic carbon normalized chemical concentration 0-10 cm (ug/gOC)